1/N expansion formalism for high-spin states

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Abstract

The $1/N$ expansion solutions for the interacting boson model are extended to higher orders using computer algebra. The analytic results are compared with those obtained from an exact diagonalization of the Hamiltonian and are shown to be very accurate. The extended formulas for level energies and E2 transitions will be useful in the analysis of high-spin states in both normal and superdeformed nuclei.

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Application of the interacting boson model [1] (IBM) to the high-spin states of normal and superdeformed nuclei has been rather slow, and certainly not commensurate with the current experimental activity in this field. The reasons for this are i) the necessity of including g bosons in the basis in addition to the usual s and d bosons, and ii) the need to include broken pairs (quasi-particles) in the basis if backbending occurs. In this work, we address the former problem and refer to Ref. [2] for recent developments in the latter. The importance of g bosons has been well established in studies involving low-lying levels of deformed nuclei (see Refs. [3, 4] for reviews). There are also many experiments on high-spin states where results are compared to the *sd*-IBM calculations showing its inadequacy. The difficulty with performing *sdg*-IBM calculations for deformed nuclei (with boson numbers $N = 12 - 16$) is that the basis space is too large, and numerical diagonalization of a Hamiltonian is not possible even on a supercomputer. Therefore various truncation schemes have been devised. These schemes are geared towards reproducing the low-lying spectrum and can not be expected to give reliable results for the high-spin states. The situation gets even worse in the case of superdeformed nuclei where recent microscopic studies have shown that the number of bosons is around $N = 30 - 40$ [5, 6], which renders any attempt to numerical diagonalization futile.

A more promising approach is to use the angular momentu"m projected mean field theory which leads to a $1/N$ expansion for all matrix elements (m.e.) of interest [7]. Initial calculations in the $1/N$ expansion formalism were restricted to order $1/N^2$ which was sufficient for low-spin ($L < N$) phenomenology. For an accurate description of high-spin properties (e.g. dynamic moments of inertia), however, one needs to include terms up to order $1/N^6$ (note that these terms actually go as $(L/N)^6$, and are not small for high-spin states). Hand calculation of m.e. to such high orders is impractical and has never been attempted. Recent advances in computer algebra have finally broken this impasse. The purpose of this letter is to report on the results of such a $1/N$ expansion calculation facilitated by the Mathematica software [8]. Applications are made to the superdeformed bands in Hg isotopes.

We consider a general formulation of the IBM and introduce the boson creation

and annihilation operators $b^\dagger_{l\mu}, b_{l\mu}$ with $l = 0, 2, 4, \ldots$. The ground band can be written as a condensate of intrinsic bosons as

$$|N, \mathbf{x}\rangle = (N!)^{-1/2}(b^\dagger)^N|0\rangle, \quad b^\dagger = \sum_l x_l b^\dagger_{l0}, \tag{1}$$

where x_l are the normalized boson mean fields which are associated with the deformation parameters of the system. Here we assume that the system is axially symmetric, which is a good approximation as will be seen later. The other bands can be obtained from the ground band by acting with the orthogonal intrinsic boson operators. A general boson Hamiltonian with one- and two-body terms is given by

$$\begin{aligned} H &= \sum_l \varepsilon_l \hat{n}_l + \sum_{k=0}^{2l_{\max}} \kappa_k T^{(k)} \cdot T^{(k)}, \\ \hat{n}_l &= \sum_\mu b^\dagger_{l\mu} b_{l\mu}, \quad T^{(k)} = \sum_{jl} t_{kjl} [b^\dagger_j \tilde{b}_l]^{(k)}, \end{aligned} \tag{2}$$

where brackets denote tensor coupling of the boson operators, $\tilde{b}_{l\mu} = (-1)^\mu b_{l-\mu}$, and $\hat{n}_l$ and $T^{(k)}$ are the boson number and multipole operators, respectively. The parameters in the model are the single boson energies ε_l, the multipole strengths κ_k, and the coefficients t_{kjl}. For consistency, the same multipole operators are used in the calculation of electromagnetic transition rates.

Matrix elements of any operator with angular momentum projection can be evaluated efficiently using boson calculus and angular momentum algebra techniques [7]. We refer to the original references for details and give here the intermediate results that form the basis of the Mathematica calculation. The exact expectation values of the number and multipole operators (2) in the ground band are given by

$$\begin{aligned} \langle \hat{n}_l \rangle_L &= \frac{N x_l^2}{F(N,L)} \sum_I \langle L0l00|I0\rangle^2 F(N-1, I), \\ \langle T^{(k)} \cdot T^{(k)} \rangle_L &= \frac{2k+1}{F(N,L)} \Big\{ N \sum_{jl} \frac{(t_{kjl} x_l)^2}{2l+1} \sum_I \langle L0l00|I0\rangle^2 F(N-1, I) \\ &\quad + N(N-1) \sum_{jlj'l'J} t_{kjl} t_{kj'l'} x_j x_l x_{j'} x_{l'} \langle j0j'0|J0\rangle \langle l0l'0|J0\rangle \\ &\quad \times \begin{Bmatrix} j & j' & J \\ l' & l & k \end{Bmatrix} \sum_I \langle L0J0|I0\rangle^2 F(N-2, I) \Big\}. \end{aligned} \tag{3}$$

Here $F(N, L)$ denotes the normalization integral which has the $1/N$ expansion [9]

$$F(N, L) = \frac{1}{N} \sum_{n=0} \frac{(-1)^n}{n!(aN)^n} \sum_{m=0}^{n} \alpha_{nm} \bar{L}^m, \tag{4}$$

where bar denotes the angular momentum eigenvalues, $\bar{L} \equiv L(L+1)$ and $a = \sum_l \bar{l} x_l^2$ represents the "average angular momentum squared" carried by a single boson. The coefficients α_{nm} in Eq. (4) have been calculated recently utilizing the Mathematica software [9]. It is clear from the expressions (3,4) that, in principle, one can evaluate these m.e. to any desired order in $1/N$ (see Ref. [7]). However, the amount of algebraic manipulation required grows exponentially with each order, and one is soon forced to give up. In contrast, Mathematica is very efficient at such "algebra crunching".

Before presenting the final results, it will be useful to comment on the general form of the m.e. of a k-body operator $\hat{O}$, and illustrate the concept of layers in the $1/N$ expansion (see Ref. [9] for more details)

$$\langle \hat{O} \rangle_L = N^k \sum_{n,m} \frac{O_{nm}}{(aN)^m} \Big(\frac{\bar{L}}{a^2 N^2} \Big)^n . \tag{5}$$

The expansion coefficients O_{nm} in Eq. (5) involve various quadratic forms of the mean fields x_l corresponding to the single-boson m.e. of $\hat{O}$ and its moments. The terms with $n + m - 1 = i$, constant, are referred as the ith layer. An expansion in layers rather than in $1/N$ is preferred on both practical and physical grounds. This is because terms in the same layer have similar forms (although they have different N dependence), while complexity of terms grows exponentially with increasing layers. For example, a complete calculation to order $1/N^6$ would involve terms belonging to the fourth, fifth and sixth layers which are very complicated yet completely unnecessary as their contribution to the m.e. is beyond the desired level of accuracy. Here we restrict ourselves to a third layer calculation of the m.e. which is found to be sufficiently accurate for description of high-spin states. For the one-body m.e. in Eq. (3), one obtains

$$\begin{aligned}
\langle \hat{n}_l \rangle_L = N x_l^2 \Big\{ 1 + \frac{1}{aN} \Big(a - \bar{l} \Big) + \frac{1}{(aN)^2} \Big(-a + a_1/2 + (1 - a_1/a)\bar{l} + \bar{l}^2/2 \Big) \\
+ \frac{1}{(aN)^3} \Big(a + 2a^2 - 7a_1/3 - a a_1 + 5a_1^2/4a - a_2/3 \\
+ (-1 - 2a + 2a_1 + 7a_1/2a - 5a_1^2/2a^2 + a_2/2a)\bar{l} \\
+ (-7/6 - a + 5a_1/4a)\bar{l}^2 - \bar{l}^3/6 \Big) \\
+ \frac{\bar{L}}{(aN)^2} \Big[(-a + \bar{l}) + \frac{1}{aN} \Big(2a + 2a^2 - 2a_1 + (-2 - 2a + 3a_1/a)\bar{l} - \bar{l}^2 \Big)
\end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{(aN)^2}\Big(-3a-12a^2-4a^3+21a_1/2+11aa_1-15a_1^2/2a+3a_2/2\\
&\qquad+(3+12a+4a^2-33a_1/2-14a_1/a+25a_1^2/2a^2-2a_2/a)\bar{l}\\
&\qquad+(7/2+11a/2-5a_1/a)\bar{l}^2+\bar{l}^3/2\Big)\Big]\\
&+\frac{\bar{L}^2}{2(aN)^4}\Big[(-a-2a^2+3a_1/2+(1+2a-2a_1/a)\bar{l}+\bar{l}^2/2)\\
&\quad+\frac{1}{aN}\Big(4a+21a^2+14a^3-16a_1-51aa_1/2+13a_1^2/a-2a_2\\
&\qquad+(-4-21a-14a^2+34a_1+20a_1/a-39a_1^2/2a^2+5a_2/2a)\bar{l}\\
&\qquad+(-4-17a/2+13a_1/2a)\bar{l}^2-\bar{l}^3/2\Big)\Big]\\
&+\frac{\bar{L}^3}{3(aN)^6}\Big[-a-6a^2-6a^3+25a_1/6+9aa_1-15a_1^2/4a+5a_2/12\\
&\qquad+(1+6a+6a^2-45a_1/4-5a_1/a+21a_1^2/4a^2-a_2/2a)\bar{l}\\
&\qquad+(5/6+9a/4-3a_1/2a)\bar{l}^2+\bar{l}^3/12\Big]\Big\},
\end{aligned}
\tag{6}
$$

where $a_n = \sum_l \bar{l}^{n+1}x_l^2$ denotes the higher moments of a. We have checked Eq. (6) against two results: i) it satisfies the number conservation, i.e. $\sum_l\langle\hat{n}_l\rangle = N$, ii) it reproduces the analytic formulas available in the SU(3) limit [1]. A similar Mathematica evaluation of the two-body m.e. in Eq. (3) gives

$$
\begin{aligned}
\langle T^{(k)}\cdot T^{(k)}\rangle_L = N^2\Big\{&U_k+\frac{1}{aN}\Big(aU_k-U_k1+aC_k\Big)\\
&+\frac{1}{(aN)^2}\Big((-2a+a_1)U_k+(1-a-a_1/a)U_{k1}+U_{k2}/2+a^2C_k-aC_{k1}\Big)\\
&+\frac{1}{(aN)^3}\Big((2a+2a^2-14a_1/3-aa_1+5a_1^2/2a-2a_2/3)U_k\\
&\qquad+(-1+a-a_1/2+7a_1/2a-5a_1^2/2a^2+a_2/2a)U_{k1}\\
&\qquad+(-7/6+5a_1/4a)U_{k2}-U_{k3}/6\\
&\qquad+(-a^2+aa_1/2)C_k+(a-a_1)C_{k1}+aC_{k2}/2\Big)\\
+\frac{\bar{L}}{(aN)^2}\Big[&-2aU_k+U_{k1}\\
&+\frac{1}{aN}\Big((4a+2a^2-4a_1)U_k+(-2+a+3a_1/a)U_{k1}-U_{k2}-a^2C_k+aC_{k1}\Big)\\
&+\frac{1}{(aN)^2}\Big((-6a-16a^2-4a^3+21a_1+15aa_1-15a_1^2/a+3a_2)U_k\\
&\qquad+(3+2a-2a^2-4a_1-14a_1/a+25a_1^2/2a^2-2a_2/a)U_{k1}\\
&\qquad+(7/2+2a-5a_1/a)U_{k2}+U_{k3}/2
\end{aligned}
$$

$$
\begin{aligned}
&+(2a^2+2a^3-2aa_1)C_k+(-2a-2a^2+3a_1)C_{k1}-aC_{k2}\Big)\Big]\\
+\frac{\bar{L}^2}{2(aN)^4}\Big[&(-2a-2a^2+3a_1)U_k+(1-2a_1/a)U_{k1}+U_{k2}/2\\
&+\frac{1}{aN}\Big((8a+30a^2+14a^3-32a_1-37aa_1+26a_1^2/a-4a_2)U_k\\
&+(-4-8a+2a^2+29a_1/2+20a_1/a-39a_1^2/2a^2+5a_2/2a)U_{k1}\\
&+(-4-9a/2+13a_1/2a)U_{k2}-U_{k3}/2\\
&+(-a^2-2a^3+3aa_1/2)C_k+(a+2a^2-2a_1)C_{k1}+aC_{k2}/2\Big)\Big]\\
+\frac{\bar{L}^3}{3(aN)^6}\Big[&(-8a-36a^2-24a^3+100a_1/3+54aa_1-30a_1^2/a+10a_2/3)U_k\\
&+(4+12a-24a_1-20a_1/a+21a_1^2/a^2-2a_2/a)U_{k1}\\
&+(10/3+6a-6a_1/a)U_{k2}+U_{k3}/3\Big]\Big\}. \qquad (7)
\end{aligned}
$$

Here the quadratic forms C_{kn} arise from normal ordering and simulate an effective one-body term

$$C_{kn}=(2k+1)\sum_{jl}\bar{l}^n(t_{kjl}x_l)^2/(2l+1), \qquad (8)$$

while U_{kn} represent the genuine two-boson interaction

$$U_{kn}=\sum_{jlj'l'I}\bar{I}^n\langle j0j'0|I0\rangle\langle l0l'0|I0\rangle\begin{Bmatrix} j & j' & I\\ l' & l & k\end{Bmatrix}t_{kjl}t_{kj'l'}x_jx_lx_{j'}x_{l'}. \qquad (9)$$

For a given multipole, these sums can be evaluated in closed form using Mathematica. For the quadrupole interaction, the first four terms needed in Eq. (7) are given by

$$
\begin{aligned}
&U_2=A^2,\quad U_{21}=(2A_1-3A)A,\\
&U_{22}=(2A_2-24A_1+18A)A+(A_{11}-A_2+7A_1)A_1+(A_{11}-A_2)^2/12,\\
&U_{23}=(2A_3-36A_2-18A_{11}+192A_1-144A)A\\
&\quad+(3A_{21}-3A_3+48A_2+24A_{11}-146A_1)A_1/2\\
&\quad-(3A_{21}-3A_3+25A_2-14A_{11})A_2/12\\
&\quad+(3A_{21}-3A_3+11A_{11})A_{11}/12, \qquad (10)
\end{aligned}
$$

where the quadratic forms A_{mn} in (10) are defined as

$$A_{mn}=\sum_{jl}\bar{j}^m\bar{l}^n\langle j0l0|20\rangle t_{2jl}x_jx_l, \qquad (11)$$

and correspond to various moments of the single-boson quadrupole m.e. (note that the zero subscripts are suppressed for convenience). The quadrupole m.e. given by (7-10) reproduces the well known Casimir eigenvalues in the SU(3) limit, hence also passes the SU(3) test.

To obtain the final energies, one has to perform variation after projection (VAP) and determine the mean fields x_l for each L. This can be done algebraically using an ansatz for x_l similar to Eq. (5), which leads to sets of linear equations for the higher order terms [7]. As the algebraic solution of the VAP equations are rather lengthy, we defer their discussion to a longer paper. Alternatively, one can determine x_l numerically using, for example, the simplex method. Both methods lead to equally accurate results. Expressions for the excited band energies are obtained in a similar manner, though they are somewhat more complicated due to contributions from orthogonality and band mixing effects, and will be given in a future paper.

The other experimentally relevant quantities in the study of high-spin states are the $E2$ transitions. In this case, the first layer results are found to be sufficiently accurate, hence higher order calculations are not necessary. For completeness, we quote the $E2$ transition m.e. in the ground band [10]

$$\begin{aligned}\langle L' \parallel T^{(2)} \parallel L\rangle = N\hat{L}\langle L0\,20|L'0\rangle\Big\{A - \frac{1}{aN}(A_1 - 3A - aA) \\ -\frac{1}{8(aN)^2}\Big[(A_2 - A_{11} - 10A_1 + 12A + 4aA)(\bar{L}' + \bar{L}) \\ -\frac{1}{6}(A_2 - A_{11} - 6A_1 + 6A)(\bar{L}' - \bar{L})^2\Big]\Big\}, \qquad (12)\end{aligned}$$

where $\hat{L} = [2L+1]^{1/2}$ and A_{mn} are defined in (11). Further expressions for in- and inter-band transitions among the ground, β and γ bands, including band mixing effects, are given in Ref. [10]. A fortran code for the $1/N$ expansion calculation of energies and $E2$ transitions is available from the authors upon request [11].

Before applying the $1/N$ expansion results, we compare them with those obtained from an exact diagonalization of the Hamiltonian [12]. For this purpose we choose two different parametrizations of *sdg*-IBM: (a) a pure quadrupole interaction which is appropriate for superdeformed states [5, 6], (b) quadrupole interaction plus a g boson energy which reflects weaker coupling of g bosons in normal deformed states. In both cases, the quadrupole parameters q_{22}, q_{24}, q_{44} are scaled from their SU(3)

values with a single factor q ($q_{02} = 1$, $q_{jl} = t_{2jl}$). The q factor gives a simple measure for the breaking of the SU(3) symmetry which is necessary for a realistic description of deformed nuclei. Of necessity, the boson number is fixed at $N = 10$, which requires some scaling of the parameters from their realistic values at larger N. Fig. 1 presents comparisons for the ground band energies. The top figures show $E_L/\bar{L}$ as a function of $\bar{L} = L(L+1)$. In case (a), the agreement between the third layer 1/N expansion calculation (solid line) and the exact results is excellent up to the maximum spin $L = 4N$. The second layer results (dotted line) start deviating from the exact ones around $L = 2N$ as do the third layer results with VBP (dashed line). In case (b), the agreement is still very good, with only a few percent difference at the very high-spin region. Here, the VBP calculation shows even larger deviations, underscoring the importance of the VAP procedure for high-spin states. In the bottom figures, we compare the dynamic moment of inertia $\mathcal{J}^{(2)}$ which is much more sensitive to changes in structure. Thus, the inadequacy of the second layer calculations, which is not very clear in the energy plots, becomes obvious in $\mathcal{J}^{(2)}$ plots. In Fig. 2, we compare the first layer results for the $E2$ transition m.e. (12) with the exact ones. The agreement is again very good up to very high-spins in both cases. The test cases discussed above indicate that the extended formalism can be applied with confidence in the spin region $L = N$-$3N$ which covers the presently available high-spin data. This, incidentally, also shows the adequacy of the axial symmetry assumption made in the beginning.

The analytic expressions derived for energies and $E2$ transitions will be useful in the study of high-spin states in both normal and superdeformed nuclei. Here, we present an application of the $1/N$ expansion formalism to superdeformation which is more topical and harder to treat by numerical diagonalization. In super IBM, as proposed by Otsuka and Honma [5, 6], normal bosons are supplemented with superdeformed bosons which correspond to the Cooper-pairs in the superdeformed potential. The number of superdeformed bosons, N_{super} is typically around 30-40, and because of large deformation, g boson effects are important. Thus, the super IBM offers a fertile ground for the application of the $1/N$ expansion. We use the energy formula (7) to describe the superdeformed bands in the Hg isotopes. The

dynamic moments of inertia, $\mathcal{J}^{(2)}$ that result from the quadrupole Hamiltonian are shown in Fig. 3. The three quadrupole parameters q_{22}, q_{24}, q_{44} are scaled from their SU(3) values with a single factor q. N_{super} is determined from microscopic calculations, [5, 6] and κ and q are fitted to the experimental data. A good description of experimental $\mathcal{J}^{(2)}$ (circles) is obtained. We note that the SU(3) limit corresponds to a rigid rotor and would give a flat line for $\mathcal{J}^{(2)}$. This happens because in the SU(3) limit, the mean fields x_l are constant (independent of L), and the structure does not change with rotation. In reality, one expects a gradual change in $\mathcal{J}^{(2)}$ due to loss of pairing. The above study shows that this can be simulated by breaking of the SU(3) symmetry which results in migration of the mean fields from s to d, and to g bosons with increasing spin. The q values obtained in the above fits indicate that this breaking is around 30%. It has been suggested that the identical band phenomenon may be due to an underlying symmetry [14, 15]. It would be of interest to pursue this suggestion by extending the present calculations to other bands and also to odd nuclei.

Another area where the $1/N$ expansion formalism could contribute significantly is the study of high-spin states in normal deformed nuclei. In many experiments on high-spin states, results were compared to the *sd*-IBM calculations with negative connotations. This is presumably due to lack of *sdg*-IBM calculations which, hopefully, will become more accessible with the analytic formulas presented here.

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Figure captions

Fig. 1. Comparison of the ground band energies (top) and dynamic moments of inertia (bottom) obtained from the $1/N$ expansion with the exact numerical results (circles). The different lines refer to the third layer calculation with VAP (solid line), third layer with VBP (dashed line), and second layer with VAP (dotted line). The VBP results for $\mathcal{J}^{(2)}$ deviate strongly from the exact ones and are not shown to avoid cluttering of the figures. The parameters of H are $\kappa = -20$ keV, $q = 0.7$ for the quadrupole interaction in both (a) and (b), and $\varepsilon_g = 500$ keV in (b).

Fig. 2. Comparison of the $E2$ transition m.e., Eq. (12) with the exact diagonalization results (circles). Solid line refers to VAP and dashed line to VBP.

Fig. 3. Comparison of the experimental dynamic moment of inertia in $^{190-194}$Hg (circles) with the super IBM calculations (solid lines). The data are from [13]. The parameters used in the fits are $N_{super} = 29, 30, 31$, $\kappa = -35, -34, -33$ keV, $q = 0.68, 0.72, 0.72$ for $^{190-192-194}$Hg, respectively.